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Radiation multigroup diffusion for refractive, lossy media in ALE3D (U)

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Multigroup Diffusion Package in ALE3D

Motivation: Simulate (rapid) heating and cooling of SiO_2 for damage mitigation on final NIF optics

General application: energy transport in refractive lossy media

Radiation, although often ignored in relatively low temperature regimes ($T < 8000$ °K) due to its low energy content, is still an efficient vehicle for energy (heat) transport and loss

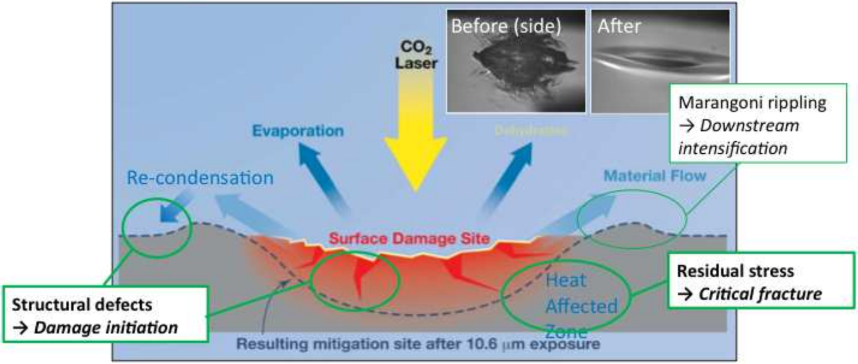
Examples:

- Campfire on a cold night
- Heat leakage through evacuated part of thermos
- Cooling of hot glass

Outline

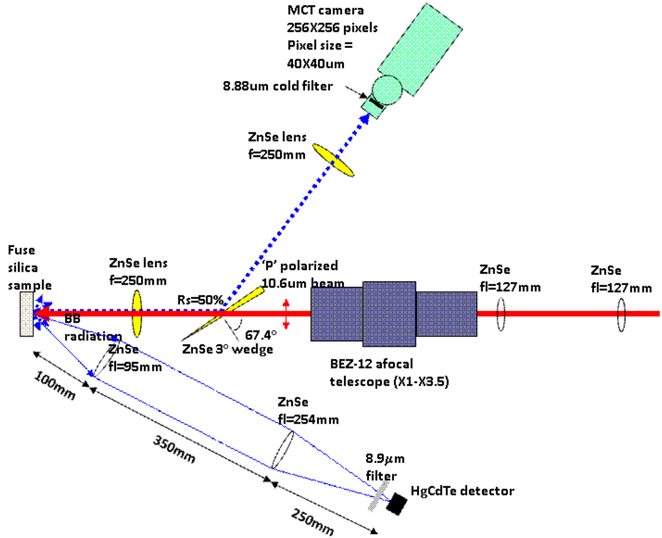
- Typical experiment
- Derivation of ALE3D radMGDiff equations
- Boundary and interface conditions
- Material properties (SiO_2)
- Results
  - 1D Slab cooling
  - 1D Comparison with Lasnex
- Ongoing work; open questions

Damage mitigation (courtesy M. Matthews *et al*)



Current LLNL work seeks to establish role of <u>viscoelastic</u> and <u>structural</u> relaxation processes in laser-based mitigation of SiO_2 surface damage

Experimental setup (courtesy S. Yang, LLNL)



Photon propagation (Pomraning)

Substitute

$\mathbf{f} = \mathbf{f}_0 \, \mathsf{exp}[i(\mathbf{k}\cdot\mathbf{r} - \omega t)], \quad \omega = \omega_r(\mathbf{r},\mathbf{k},t) + i\,\omega_i(\mathbf{r},\mathbf{k},t)$

into Maxwell's equations. Get...

Motion of wave packet (Hamilton's equations) $\Rightarrow$

Equations of photon propagation ($\omega_r = 2\pi\nu$):

$$\begin{aligned} d\mathbf{r}/ds &= \mathbf{\Omega} \\ d\mathbf{\Omega}/ds &= (1/n)\,[\nabla n - \mathbf{\Omega}\,(\mathbf{\Omega}\cdot\nabla n)] \\ d\nu/ds &= -(\nu/c)\,\partial_t n \end{aligned}$$

$d\mathbf{r}/dt = v_g\,\mathbf{\Omega}$

Refractive index $n \doteq ck_w/\omega$, $k_w = |\mathbf{k}|$

Homogeneous medium: $(\nabla n,\, \partial_t n = 0) \Rightarrow (d\nu/ds,\, d\mathbf{\Omega}/ds = 0)$

Derivation of ALE3D diffusion equations

Add emission, absorption to Pomraning's streaming operator
Assume homogeneous medium ($\nabla n = 0 = \partial_t n$)

$$n^2 \left[(1/v_g)\,\partial_t (I/n^2) + \mathbf{\Omega} \cdot \nabla (I/n^2) \right] = \kappa \left[n^2\, \mathcal{B}_\nu(T) - I \right]$$

$$\mathcal{B}_\nu(T) = \frac{2h\nu^3/c^2}{\exp(h\nu/k_B T) - 1}$$

$v_g \doteq$ group speed; phase speed $v_p \doteq c/n$
$1/v_g \doteq (\partial k_w/\partial \omega) = (n + \nu \partial_\nu n)/c \doteq 1/v_p + (\nu \partial_\nu n)/c$

$h,\ k_B =$ Planck, Boltzmann constants

opacity $\kappa = 4\pi k/\lambda$, wavelength $\lambda = c/\nu$

$(n,\ k) \doteq$ dimensionless (refractive, absorption) indexes

Intensity moments

Spectral energy density E, flux $\mathbf{F}$, and pressure tensor $\overline{\overline{\mathsf{P}}}$:

$$\begin{aligned} E &\doteq (1/v_g) \int_{4\pi} d\omega\, I \\ \mathbf{F} &\doteq \int_{4\pi} d\omega\, \mathbf{\Omega}\, I \\ \overline{\overline{\mathsf{P}}} &\doteq (1/v_g) \int_{4\pi} d\omega\, \mathbf{\Omega}\,\mathbf{\Omega}\, I\,, \end{aligned}$$

Take moments of intensity equation

Close system: ignore $\partial_t(\mathbf{F}/n^2)$ and $\overline{\overline{\mathsf{P}}} \rightarrow (E/3)\,\overline{\overline{\mathsf{I}}}$

ALE3D RadMGDiff module solves

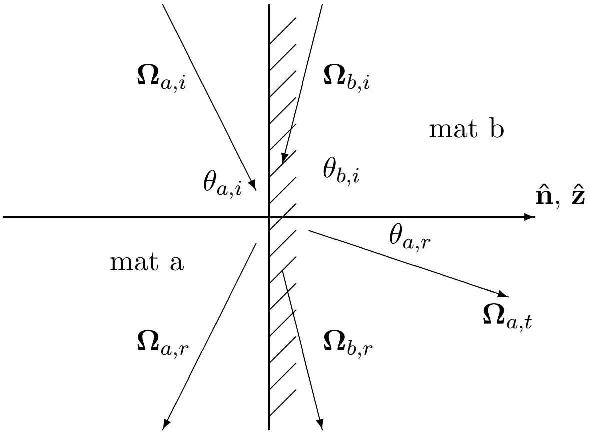
$$\partial_t E = \nabla \cdot \frac{v_g}{3\kappa} \nabla E + \kappa \, v_g \left[4\pi \, n^2 \, \mathcal{B}_\nu(T)/v_g - E \right]$$

$$\rho c_{\mathsf{v}} \, \partial_t T = \underbrace{\nabla \cdot k_m \nabla T + S}_{\mathsf{op-split}} - \int_{\nu_0}^{\infty} d\nu \, \kappa \, v_g \left[4\pi \, n^2 \, \mathcal{B}_\nu(T)/v_g - E \right]$$

$v_g = v_g(\nu, n)$; (until have better data, $v_g \doteq v_p = c/n$)
$n = n(\nu) \doteq$ refractive index
$k = k(\nu) \doteq$ absorption index; $\kappa = 4\pi k/\lambda = 4\pi k\nu/c$;
$S =$ external energy source (laser)
$\nu_0 \doteq$ upper bound of *opaque* interval (Larsen *et al*)

Usual multigroup diffusion: $v_g \rightarrow c$, $n \rightarrow 1$
LTE: E depends on T and material-dependent n, v_g

Boundary & (Interior) Interface conditions



$\mathbf{\Omega}_{a,i} \rightarrow \mathbf{\Omega}_{a,r} + \mathbf{\Omega}_{a,t}$
$\mathbf{\Omega}_{b,i} \rightarrow \mathbf{\Omega}_{b,r}$ (total reflection)

Reflectivity, boundary, interface conditions

Reflected fraction of incident intensity $R(\mu)$ obtained from Snell's law(s), energy conservation, Maxwell's equations

Snell's law(s) relate incident, refracted angles, material indexes n, k across interface

In lossy media ($k \neq 0$), Snell's law is complicated (complex)

Boundary conditions (Larsen *et al*)

At boundary, in medium,

$$I = I_b(\mathbf{\Omega}) = I_{b,t}(\mathbf{\Omega}) + I_{b,r}(\mathbf{\Omega}) \tag{1}$$

"Transmitted" radiation:

$$I_{b,t}(\mathbf{\Omega}) = [\,1 - R(\mu)\,]\,\mathcal{B}_\nu(T_a)$$

"Reflected" radiation:

$$I_{b,r}(\mathbf{\Omega}) = R(\mu)\,I(\mathbf{\Omega}')\,, \quad \mathbf{\Omega}' = \mathbf{\Omega} - 2\,(\hat{\mathbf{n}}\cdot\mathbf{\Omega})\,\hat{\mathbf{n}}$$

For diffusion, satisfy Eq.(1) in integral sense:

$$2\pi \int_0^1 d\mu\,\mu\,(I - I_b) = 0$$

Boundary conditions (air-glass interface)

$$E + \left(\frac{1+3r_2}{1-2r_1}\right)\left(\frac{2}{3\kappa}\right)(\hat{\mathbf{n}}\cdot\nabla E) = 4\pi\, n^2\,\mathcal{B}_\nu(T_a)/v_g$$

$$\hat{\mathbf{n}}\cdot(k_m\nabla T) = h_m(T_a - T) + \pi\,(1-2r_1)\,n_0^2 \int_0^{\nu_0} d\nu\,[\mathcal{B}_\nu(T_a) - \mathcal{B}_\nu(T)]$$

T_a = external temperature
r_1, r_2 = moments of reflectivity $R(\nu, n, k)$, $r_j \doteq \int_0^1 d\mu\,\mu^j\,R(\mu)$
h_m = convection coefficient
$(0,\, \nu_0) \doteq$ *opaque* interval (strong coupling) (Larsen *et al*)

Conventional Milne conditions: $r_1,\, r_2 \to 0$

(Interior) interface conditions (materials a, b) (WIP)

Diffusion approximation:

$$I(\mathbf{\Omega}) = \frac{v_g}{4\pi} \left[E + 3\,\mathbf{\Omega} \cdot \left(\frac{1}{3\kappa} \nabla E \right) \right]$$

Integrate over hemisphere in side b:

$$\frac{v_g}{n^2} \left[E - \left(\frac{1+3r_2}{1-2r_1} \right) \left(\frac{2}{3\kappa} \right) (\hat{\mathbf{n}} \cdot \nabla E) \right] =$$
$$\frac{v_{g,a}}{n_a^2} \left[E_a - \left(\frac{1-3r_{2,a}}{1-2r_{1,a}} \right) \left(\frac{2}{3\kappa_a} \right) (\hat{\mathbf{n}} \cdot \nabla E_a) \right]$$

In corresponding hemispheres, $r_j = \int_0^1 d\mu\, \mu^j\, R(\mu)$

Interface conditions (materials a, b) (WIP)

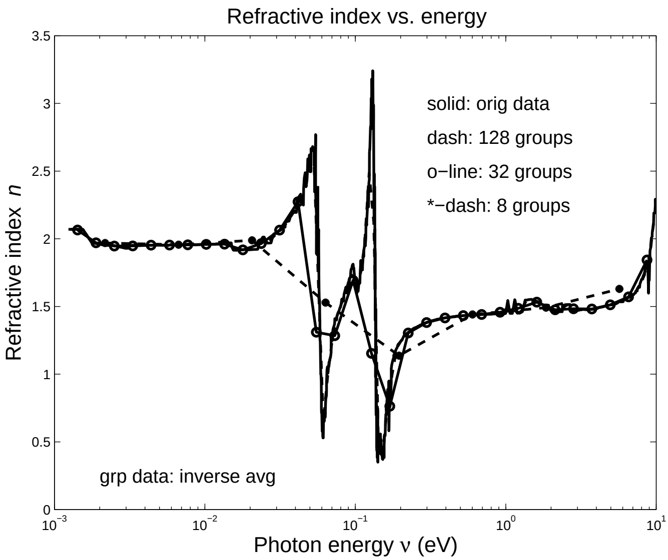
Radiation interface condition of form:

$$A_a E_a + B_a \hat{\mathbf{n}} \cdot \nabla E_a = A_b E_b + B_b \hat{\mathbf{n}} \cdot \nabla E_b$$

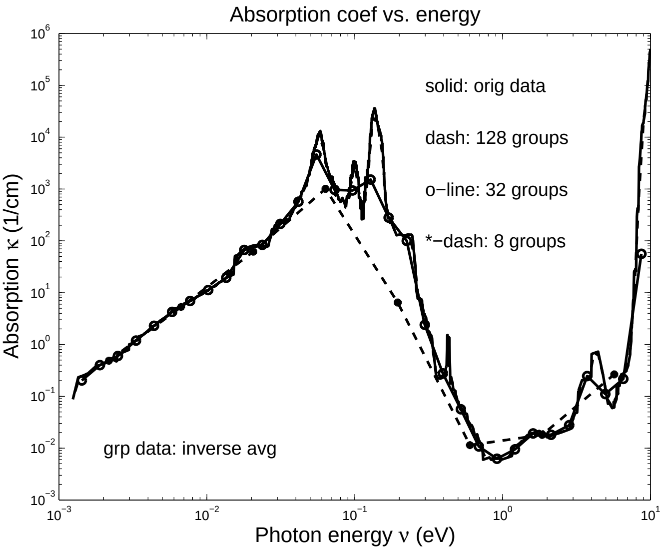
Challenge: As $(n_a,\, k_a) \to (n_b,\, k_b)$, ensure discretization of interface condition satisfies:

$$\partial_t E = \nabla \cdot \frac{v_g}{3\kappa} \nabla E + \kappa\, v_g \left[\, 4\pi\, n^2\, \mathcal{B}_\nu(T)/v_g - E \,\right]$$

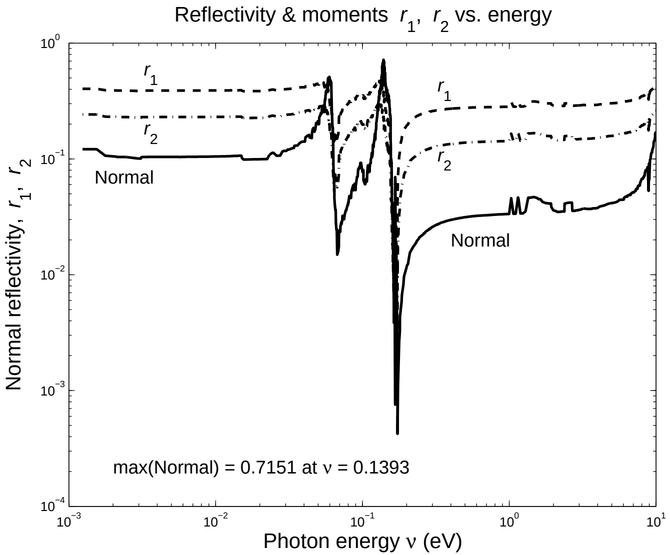
T equation: $\rho c_\mathsf{v}\, \partial_t T = \nabla \cdot k_m \nabla T$, unaffected by interface



SiO_2 room temperature refraction index (Kitamura)



SiO_2 room temperature opacity (from Kitamura data)



SiO_2 room temperature normal reflectivity and moments

Results: RadCool test problem

- Bouchut parameters:

  $\rho c_{\mathsf{v}} = 2.201 \cdot 10^7$ (erg/cc °K)

  $k_m = 2.201 \cdot 10^5$ (erg/cm sec °K)

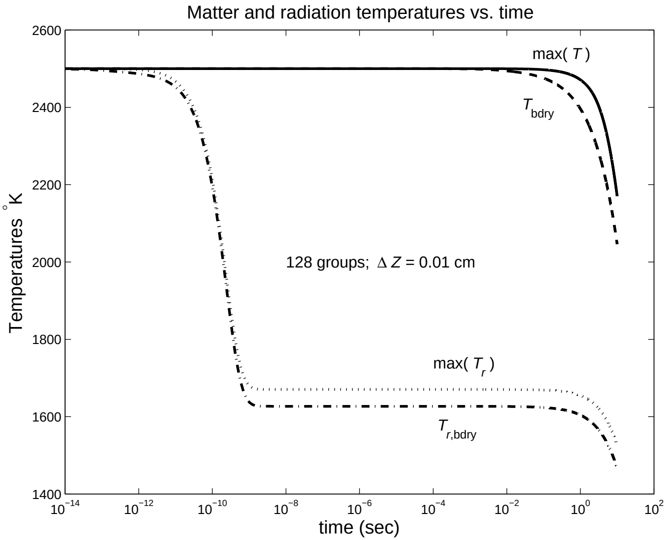
- 1D: $0 < Z < 0.5$ cm
- Initial conditions: $T = T_r = 2500\,^\circ\mathrm{K}$
- Boundary conditions:

  $Z = 0.0$: $T_a = 298.15\,^\circ\mathrm{K}$ (air)

  $Z = 0.5$: symmetry

- Display timehist: max & bdry T and T_r

  $T_r^4 \doteq \frac{1}{4\sigma} \sum_{i=1}^{G} v_i\, E_i / n_i^2$, $\sigma =$ Stefan-Boltzmann const



RadCool problem; matter, radiation temperature time histories

On retaining $\partial_t E$...

For low T applications, $\partial_t E$ is often ignored (Larsen *et al*)
$\rho c_v \gg 4aT_r^3$ and Δt is "large" ($c = \infty$ assumption)

$\partial_t E$ may be of same order as other terms in E equation:

$\nu = 0.12$ eV, $\kappa \approx 4 \cdot 10^4$, cm^{-1}

$\Delta t = 10^{-7}$ s, $v_g \sim c$, $\nabla \sim 1/\ell$, $\ell =$ specimen size (1 cm)

$(\partial_t E : \nabla \cdot \frac{v_g}{3\kappa} \nabla E) \sim (E/\Delta t : c\,E/3\kappa\ell^2) \sim (40 : 1)$

RadCool test problem; effect of retaining $\partial_t E$

Define $M_{t,r}$ multiplier of $\partial_t E$ term

Effect of $M_{t,r}$ on max radiation temperature $\mathsf{max}(T_r)$:

t	10^{-15}	10^{-11}	10^{-10}	10^{-9}	10^{-8}
$M_{t,r} = 1.0$	2500	2464	2169	1560	1548
$M_{t,r} = 10^{-14}$	1548	1548	1548	1548	1548

$\partial_t E$ enables monitoring rapid changes in thermal fluxes

Results: RadCool2 problem; LASNEX vs. ALE3D

Two "materials"

- Mat1: $0.0 < Z < 0.5$ cm; Bouchut parameters ρc_{v}, k_m
- Mat2: $0.5 < Z < 1.0$ cm; Bouchut parameters $\times 10^{-1}$
- For Mat2, n, k vary linearly w/ T; (100–5000), 10x increase
- Initial conditions: $T = T_r = 2500\,^\circ\mathrm{K}$
- Boundary conditions: $T_a = 298.15\,^\circ\mathrm{K}$

RadCool2 Test problem; comparison of runs

	LAS	A3D$_{(n=1)}$
$\max(T_m)$	2477.3	2478.5
$\max(T_r)$	1555.6	1549.4
$T_{m,l}$	2428.8	2404.2
$T_{r,l}$	1424.5	1411.3
$T_{m,r}$	1687.0	1578.7
$T_{r,r}$	1328.9	1286.2
$\mathrm{E}_m \cdot 10^{-3}$	1.4704	1.4675
$\mathrm{E}_r \cdot 10^{-15}$	1.9469	1.9194
$\mathrm{E}_c \cdot 10^{-5}$	4.2706	4.5668

Table: Slab cooling problem; ALE3D, LASNEX comparison; 16 groups; $t = 1$ s; maximum, left-side, right-side temperatures (°K); matter, radiation, coupled energies (J/radian)

Open questions

Are interface conditions limiting case of Pomraning's equations for spatially varying n, k?

- Interface condition has abrupt change in n, k
- Pomraning assumes weak dependence $\omega(\mathbf{r}, t)$
- $\omega = ck_w/n$, (k_w = wave vector)

Include ∇n term? $[\nabla n = (\partial n/\partial T)\, \nabla T]$

Include $d\nu/ds$? $[= -(\nu/c)\, \partial_t n = -(\nu/c)\, (\partial n/\partial T)\, (\partial T/\partial t)]$

If $\partial k/\partial T \neq 0 \Rightarrow \partial n/\partial T \neq 0 \ldots$

Temperature dependence of k

$k(\nu)$ has a strong T dependence for certain ν (λ)

McLachlan, Meyer (M&M,1987): $k = a(\nu) + b(\nu)\,T$

M&M give a, b at select wavelengths: $\lambda \in (9.6,\ 10.6)$ μm

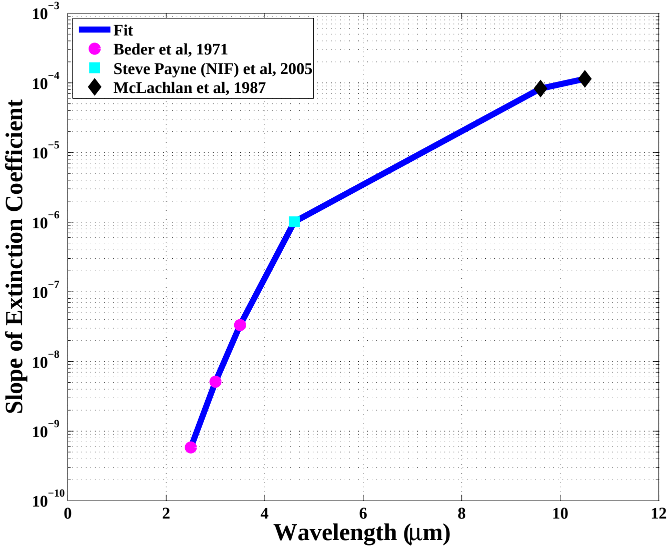
Yang et al, (LLNL, 2009) present a, b for $\lambda = 4.6$ μm

λ	10.6	4.6
ν (eV)	0.117	0.270
$a(\nu)$	$1.82 \cdot 10^{-2}$	$2.45 \cdot 10^{-4}$
$b(\nu)$	$1.01 \cdot 10^{-4}$	$6.39 \cdot 10^{-7}$
$\kappa^{-1}_{T=25}$	40.7	1403
$\kappa^{-1}_{T=1800}$	4.22	262

T in ($^\circ$C), κ^{-1} in (μm)

For $\lambda = 10.6\,\mu$m, k has $10\times$ variation over 1800 degrees!

$k(\lambda)$ Temperature dependence



Coefficient b vs. wavelength in expression: $k = a(\lambda) + b(\lambda)\,T$

Refraction n, absorption k indexes are related

Cauchy integral theorem and assumptions:

- $\lim_{\nu\to\infty}(n-1) < 1/\nu$
- $\lim_{\nu\to\infty}(k) < 1/\nu$,

yield Kramers–Kronig relation:

$$\begin{aligned} n(\nu) &= 1 + \frac{2}{\pi}\,\mathcal{P}\int_0^\infty \frac{\nu'\,k(\nu')\,d\nu'}{(\nu')^2-\nu^2} \\ k(\nu) &= \frac{-2\nu}{\pi}\,\mathcal{P}\int_0^\infty \frac{n(\nu')\,d\nu'}{(\nu')^2-\nu^2} \end{aligned}$$

If k depends on temperature, so does n

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That's all, folks

Results: 2D Laser irradiated disk (Vignes, Stölken)

Domain: $0 \leq R \leq 2.5$, $0 \leq Z \leq 1.0$ cm

Compare runs: Heat Conduction only, HC+rad

Radiation: 32 groups, Kitamura "cold" opacities

Laser source: $I_{\mathsf{lzr}} \exp(-\kappa_{\nu,\mathsf{lzr}} Z)$

$\lambda_{\mathsf{lzr}} = 10.6\,\mu\text{m}$, or $\lambda_{\mathsf{lzr}} = 4.6\,\mu\text{m}$

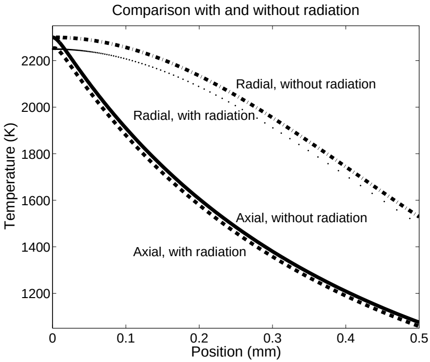
Constant material pties:

$c_{\mathsf{v}} = 10^3$ (J/kg °K), $k_m = 2.2$ (W/m °K)

$\kappa_{\mathsf{lzr}}^{-1} = 6.7\,\mu\text{m}$ ($\lambda = 10.6$), $\kappa_{\mathsf{lzr}}^{-1} = 516\,\mu\text{m}$ ($\lambda = 4.6$)

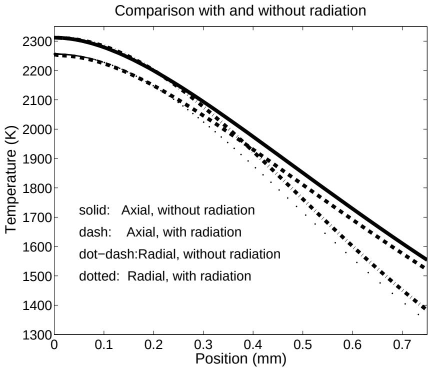
Constant material properties

$\lambda = 10.6\,\mu\mathrm{m}$



50K difference in $\max(T)$

$\lambda = 4.6\,\mu\mathrm{m}$



60K difference in $\max(T)$